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NOTE ON THE DIFFERENCE BETWEEN THE a-CYCLIC AND c-CYCLIC VERSION OF THE *XY* MODEL

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The transverse susceptibility of the c-cyclic version of the one-dimensional *XY* model with respect to an infinitesimal magnetic field in the *x*-direction is investigated in more detail. Special attention is paid to the c-cyclic version of the one-dimensional Ising model. The c-cyclic susceptibility χ_{xx} is evaluated explicitly. The autocorrelation function of the magnetization M_x turns out to be time dependent in the c-cyclic Ising model.

1. Introduction

The one-dimensional *XY* model has been introduced by Lieb, Schultz and Mattis[1]). Katsura[2]) evaluated the free energy and the non-equilibrium properties were treated by Niemeyer[3]). Since then the *XY* model has been investigated extensively. Most treatments use the so-called c-cyclic version, which can be diagonalized exactly in terms of fermion operators. In many cases such as in the calculation of time-dependent correlations between *z*-components of spins, the c-cyclic model can be shown to produce exact results in the thermodynamic limit[4-6]).

A more complicated quantity is the transverse susceptibility with respect to an infinitesimal magnetic field B_x in the x direction, *i.e.*

$$\chi = \lim_{N\to\infty} \lim_{B_x\to 0} (\beta N)^{-1} \frac{\partial^2}{\partial B_x^2} \ln \langle e^{-\beta(\mathscr{H} - B_x M_x)} \rangle \tag{1a}$$

$$= \lim_{N\to\infty} N^{-1} \sum_{k,j=1}^{N} \int_0^\beta d\tau \, \langle \varrho \, e^{\tau\mathscr{H}} S_j^x \, e^{-\tau\mathscr{H}} S_k^x \rangle, \tag{1b}$$

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where $\varrho = e^{-\beta\mathscr{H}} \langle e^{-\beta\mathscr{H}} \rangle^{-1}$ is the density operator corresponding to the hamiltonian $\mathscr{H}$ in the absence of B_x, $M_x = \sum_{j=1}^{N} S_j^x$ is the x-component of the magnetization and $\langle 0 \rangle \equiv \mathrm{Tr}\, 0$ for an arbitrary operator 0.

In ref. 7 we have given a high-temperature expansion up to order β^6 for the transverse susceptibility χ_a of the one-dimensional a-cyclic XY model described by the hamiltonian $\mathscr{H} = \mathscr{H}_a$, where

$$\mathscr{H}_a = \sum_{j=1}^{N} \{(1 + \gamma) S_j^x S_{j+1}^x + (1 - \gamma) S_j^y S_{j+1}^y - B_z S_j^z\} \quad (S_{N+1} \equiv S_1). \tag{2}$$

Here γ is the anisotropy parameter and B_z is a magnetic field in the z-direction.

Using the Jordan–Wigner transformation

$$\alpha_j = \left\{\prod_{k=1}^{j-1} P_k\right\} S_j^x \sqrt{2}, \qquad \beta_j = -\left\{\prod_{k=1}^{j-1} P_k\right\} S_j^y \sqrt{2}, \tag{3}$$

where

$$P_k = (2/\mathrm{i})\, \alpha_k \beta_k = -2S_k^z, \tag{4}$$

and where the α's and β's are hermitean operators satisfying the anticommutation relations

$$\{\alpha_i, \alpha_j\} = \{\beta_i, \beta_j\} = \delta_{ij}, \qquad \{\alpha_i, \beta_j\} = 0; \tag{5}$$

the hamiltonian $\mathscr{H}_a$ can be written[5])

$$\mathscr{H}_a = \mathscr{H}_c + \tfrac{1}{2} h (P + 1). \tag{6}$$

Here $\mathscr{H}_c$ is the c-cyclic hamiltonian given by

$$\mathscr{H}_c = \sum_{j=1}^{N} \{\tfrac{1}{2}(1 + \gamma)\, \alpha_{j+1}\beta_j + \tfrac{1}{2}(1 - \gamma)\, \alpha_j \beta_{j+1} - \mathrm{i} B_z \alpha_j \beta_j\},$$
$$(\alpha_{N+1} \equiv \alpha_1,\ \beta_{N+1} \equiv \beta_1). \tag{7}$$

The operator P is the product of all Jordan–Wigner factors $P = \prod_{j=1}^{N} P_j$ and the operator h contains the operators (3) relative to site 1 and N, *i.e.*,

$$h = -\mathrm{i}(1 + \gamma)\, \alpha_1 \beta_N - \mathrm{i}(1 - \gamma)\, \alpha_N \beta_1$$
$$= \{2(1 + \gamma) S_1^x S_N^x + 2(1 - \gamma) S_1^y S_N^y\} P. \tag{8}$$

Using (6), (8) and the trivial relation $P^2 = 1$, $\mathscr{H}_c$ can be expressed by

$$\mathscr{H}_c = \mathscr{H}_a - \{(1 + \gamma) S_1^x S_N^x + (1 - \gamma) S_1^y S_N^y\}(1 + P). \tag{9}$$

In ref. 7, the averages in eq. (16) with respect to the hamiltonian $\mathscr{H}_a$ were expressed in terms of averages with respect to the c-cyclic hamiltonian $\mathscr{H}_c$ (and also its c-anticyclic counter part) using a projection operator technique as in ref. 5. A difficulty was the occurrence of an operator containing the c-cyclic as well as the c-anticyclic hamiltonian $\mathscr{H}_{ac} \equiv \mathscr{H}_c + h$. The c-cyclic averages were evaluated using the thermodynamic Wick theorem due to Bloch and de Dominicis[8]).

We also investigated the spin correlation functions in eq. (1b) with respect to the c-cyclic hamiltonian $\mathscr{H}_c$. As a result of a high-temperature expansion we obtained the relation, *cf.* eq. (7.19) of ref. 7,

$$\langle \varrho_c \, e^{\tau \mathscr{H}_c} S_j^x \, e^{-\tau \mathscr{H}_c} S_{j+p}^x \rangle = \langle \varrho_a \, e^{\tau \mathscr{H}_a} S_j^x \, e^{-\tau \mathscr{H}_a} S_{j+p}^x \rangle \cdot \langle \varrho_c \, e^{\tau \mathscr{H}_c} e^{-\tau(\mathscr{H}_c + h)} \rangle, \quad (10)$$

where ϱ_c and ϱ_a are the density operators corresponding to $\mathscr{H}_c$ and $\mathscr{H}_a$ resp. Eq. (10) is valid, up to an arbitrary order in β, for sufficiently large values of j and $N - j - p$.

From (10) one can expect the inequality

$$\chi_c \neq \chi_a, \quad (11)$$

where χ_c and χ_a are the c-cyclic and a-cyclic susceptibilities, which can be obtained from eq. (1b) by substituting $\mathscr{H} = \mathscr{H}_c$ and $\mathscr{H} = \mathscr{H}_a$ respectively. (In fact, χ_c was evaluated up to order β^4, *cf.* eq. (7.23) of ref. 7.)

The inequality (11) is only valid, if one first takes the limit $B_x \to 0$ and the thermodynamic limit $N \to \infty$ afterwards. If one defines "thermodynamic" susceptibilities $\tilde{\chi}_c$ and $\tilde{\chi}_a$ by interchanging the two limits in eq. (1a), then both susceptibilities should be equal. This is obvious from the relation

$$f(\mathscr{H}_c - B_x M_x) = f(\mathscr{H}_a - B_x M_x) \quad (12)$$

for the free energy per particle $f(\mathscr{H}) = \lim N^{-1} F(\mathscr{H})$, $F(\mathscr{H}) = -\beta^{-1} \ln \langle e^{-\beta \mathscr{H}} \rangle$, corresponding to the hamiltonians $\mathscr{H} = \mathscr{H}_c - B_x M_x$ and $\mathscr{H} = \mathscr{H}_a - B_x M_x$. Eq. (12) is an immediate consequence of a special case of the Bogoliubov inequality[9])

$$F(\mathscr{H}_0) - \|\mathscr{H}_1\| \leqslant F(\mathscr{H}_0 + \mathscr{H}_1) \leqslant F(\mathscr{H}_0) + \|\mathscr{H}_1\|, \quad (13)$$

where $\|0\| = \sup |(x, 0x)| \, (x, x)^{-1}$ is the operator norm. Eq. (12) is obvious from (9) and (13), since the norm $\|(\mathscr{H}_c - \mathscr{H}_a)\|$ is finite.

Since there is no reason to doubt the validity of the relation $\chi_a = \tilde{\chi}_a$ for the a-cyclic model, eq. (11) implies that $\chi_c \neq \tilde{\chi}_c$, *i.e.* in the calculation of the susceptibility χ_{xx} for the c-cyclic chain the two limits $B_x \to 0$ and $N \to \infty$ cannot be interchanged. Note that for a direct evaluation of $\tilde{\chi}_a = \tilde{\chi}_c$ one should know the free energy of an XY chain in the presence of B_x. In ref. 7 we calculated χ_{xx} for a finite chain in the limiting case $B_x \to 0$, taking the thermodynamic limit afterwards. The inequality (11) shows that the difference between the transverse susceptibilities per particle in the absence of a field B_x for finite a-cyclic and c-cyclic chains tends to a non-vanishing value in the thermodynamic limit.

As another consequence of (10) one can expect a difference between the c-cyclic and a-cyclic autocorrelation functions of the x component of the magnetization, *i.e.*,

$$R_c(t) \neq R_a(t), \tag{14}$$

where

$$R_\varepsilon(t) \equiv \lim_{N\to\infty} N^{-1} \{\langle \varrho_\varepsilon M_x \, e^{i\mathscr{H}_\varepsilon t} \, M_x \, e^{-i\mathscr{H}_\varepsilon t}\rangle - \langle \varrho_\varepsilon M_x \rangle^2\} \qquad (\varepsilon = c, a). \tag{15}$$

In section 2 both inequalities (11) and (14) will be made more explicit for the simple case of an Ising model, where the c-cyclic quantities χ_c and $R_c(t)$ can be evaluated exactly without using high-temperature expansions or expansions in powers of t. (Of course for this particular case the free energy per spin of the a-cyclic model in the presence of a magnetic field B_x is well known. Our purpose, however, is to show that the use of the c-cyclic version leads to an expression for χ_c different from $\chi_a = \tilde{\chi}_a = \tilde{\chi}_c$.)

2. Ising model

In this section we shall evaluate the c-cyclic correlation functions

$$C_{jk}(\tau) \equiv \langle \varrho_c \, e^{\tau\mathscr{H}_c} \, S_j^x \, e^{-\tau\mathscr{H}_c} \, S_k^x \rangle \tag{16}$$

in the special case $\gamma = 1$, $B_z = 0$. The a-cyclic hamiltonian is then given by

$$\mathscr{H}_a = 2 \sum_{j=1}^{N} S_j^x S_{j+1}^x \qquad (S_{N+1}^x \equiv S_1^x). \tag{17}$$

Since the spin components S_j^x commute with $\mathscr{H}_a$, the a-cyclic time xx spin correlation functions and consequently the correlation function of M_x do not depend on time.

For the a-cyclic model we have

$$\langle \varrho_a S_j^x S_k^x \rangle = \tfrac{1}{4} \{(-\tanh \tfrac{1}{2}\beta)^{|k-j|} + (-\tanh \tfrac{1}{2}\beta)^{N-|k-j|}\} \times \{1 + (-\tanh \tfrac{1}{2}\beta)^N\}^{-1}, \tag{18}$$

$$\chi_a = \lim_{N\to\infty} \sum_{p=0}^{N-1} \beta \, \langle \varrho_a S_1^x S_{1+p}^x \rangle = \tfrac{1}{4}\beta \, e^{-\beta} = \tilde{\chi}_a = \tilde{\chi}_c, \tag{19}$$

$$R_a(t) = \tfrac{1}{4} e^{-\beta}. \tag{20}$$

The equality $\tilde{\chi}_a = \frac{1}{4}\beta\, e^{-\beta}$ is well known; the equality $\tilde{\chi}_a = \tilde{\chi}_c$ has been justified in section 1.

The hamiltonian of the c-cyclic version of the Ising model reads

$$\mathscr{H}_c = \mathscr{H}_a - 2S_1^x S_N^x (1 + P). \tag{21}$$

In the evaluation of the r.h.s. of (16) use will be made of the (anti) commutation relations

$$\begin{aligned} &\{P, S_k^x\} = 0, \qquad [\mathscr{H}_a, S_k^x] = 0, \\ &[S_1^x S_N^x (1 \pm P), \mathscr{H}_c] = 0 \end{aligned} \tag{22}$$

and eq. (8) for the special case $\gamma = 1$, $B = 0$. Then

$$\begin{aligned} C_{jk}(\tau) &= \langle \varrho_c\, e^{-2\tau S_1{}^x S_N{}^x(1+P)}\, e^{\tau\mathscr{H}_a}\, S_j^x\, e^{-\tau\mathscr{H}_a}\, S_k^x\, e^{2\tau S_1{}^x S_N{}^x(1-P)} \rangle \\ &= \langle \varrho_c\, e^{-4\tau S_1{}^x S_N{}^x P}\, S_j^x S_k^x \rangle = \langle \varrho_c\, e^{-h\tau}\, S_j^x S_k^x \rangle \\ &= C_{kj}(\tau). \end{aligned} \tag{23}$$

The operator $e^{-h\tau}$, for $\gamma = 1$, $B = 0$, can be written

$$e^{-h\tau} = \cosh\tau - 4S_1^x S_N^x P \sinh\tau = \cosh\tau + 2i\alpha_1\beta_N \sinh\tau. \tag{24}$$

Using the Jordan–Wigner transformation (3), the anti-commutation relations (5) and eq. (24) we obtain, $(p \geq 0)$,

$$C_{jj+p} = \tfrac{1}{4} \langle \varrho_c (\cosh\tau + 2i\alpha_1\beta_N \sinh\tau)\, (2/i)^p \prod_{k=j}^{j+p-1} (\beta_k \alpha_{k+1}) \rangle. \tag{25}$$

The r.h.s. of (25) can be evaluated using the thermodynamic Wick theorem and the relations, *cf.* eqs. (2.25), (2.29), (3.17)–(3.19) of ref. 7,

$$\begin{aligned} &\langle \varrho_c \alpha_j \alpha_k \rangle = \langle \varrho_c \beta_j \beta_k \rangle = \tfrac{1}{2}\delta_{jk}, \\ &\langle \varrho_c \alpha_j \beta_k \rangle = \tfrac{1}{2} i \,(\tanh \tfrac{1}{2}\beta)\, \delta_{k,j-1}. \end{aligned} \tag{26}$$

As a result we obtain

$$C_{jj+p}(\tau) = \tfrac{1}{4} (-\tanh\tfrac{1}{2}\beta)^p (\cosh\tau - \sinh\tau \tanh\tfrac{1}{2}\beta). \tag{27}$$

The second factor in eq. (27), which is equal to $\langle \varrho_c e^{-h\tau} \rangle$ can also be obtained from the second factor on the r.h.s. of eq. (10) in the special case that $\gamma = 1$, $B = 0$, so that $[\mathscr{H}_c, h] = 0$. Note that eq. (27) is also valid for a finite chain and that the correlation function is independent of j. This is not true in the general case of the XY model.

From eq. (27) we obtain immediately the c-cyclic susceptibility in the thermodynamic limit

$$\chi_c = \int_0^\beta d\tau \left\{ C_{jj}(\tau) + \sum_{p=1}^{\infty} C_{jj+p}(\tau) \right\}$$

$$= 2\,(\tanh \tfrac{1}{2}\beta) \left\{ \tfrac{1}{4} + \tfrac{1}{2} \sum_{p=1}^{\infty} (-\tanh \tfrac{1}{2}\beta)^p \right\} = \chi_a 2\beta^{-1} \tanh \tfrac{1}{2}\beta, \tag{28}$$

which is clearly different from $\chi_a = \tilde{\chi}_a = \tilde{\chi}_c$. Substituting $\tau = -\mathrm{i}t$ in eq. (27), we find

$$\langle \varrho_c S_j^x \,\mathrm{e}^{\mathrm{i}t\mathscr{H}_c}\, S_k^x \,\mathrm{e}^{-\mathrm{i}t\mathscr{H}_c} \rangle = \tfrac{1}{4}\,(-\tanh \tfrac{1}{2}\beta)^{|k-j|} \,(\cos t + \mathrm{i} \sin t \tanh \tfrac{1}{2}\beta). \tag{29}$$

The validity for $k < j$ can be seen by taking the hermitean conjugate of both members of the corresponding equation for $k > j$. As a result the auto-correlation function of the x component of the magnetization is given by

$$R_c(t) = \tfrac{1}{4}\,\mathrm{e}^{-\beta}\,(\cos t + \mathrm{i} \sin t \tanh \tfrac{1}{2}\beta). \tag{30}$$

As a result of using the c-cyclic version the time auto-correlation function of M_x is no longer a constant but depends on time. The time average of $R_c(t)$ vanishes (also in the case of the finite c-cyclic Ising model). Hence, the magnetization M_x is an *ergodic operator* in the c-cyclic Ising model. (Both for finite N and in the limit $N \to \infty$.) In the finite and infinite a-cyclic Ising chain M_x is *not* an ergodic operator, since in the absence of B_x the microcanonical and canonical averages of M_x vanish, whereas the time average of $R_a(t)$ is given by (20).

3. Remark

So far we have restricted ourselves to the c-cyclic version of the Ising model. For the c-anticyclic version, which is defined by the hamiltonian

$$\mathscr{H}_{ac} \equiv \mathscr{H}_c + h = \mathscr{H}_a - 2S_1^x S_N^x\,(1 - P), \tag{31}$$

the correlation functions C'_{jj+p} are also given by the r.h.s. of (27), *i.e.*,

$$C'_{jj+p}(\tau) \equiv \langle \varrho_{ac}\,\mathrm{e}^{\tau\mathscr{H}_{ac}}\, S_j^x\, \mathrm{e}^{-\tau\mathscr{H}_{ac}}\, S_{j+p}^x \rangle = C_{jj+p}(\tau). \tag{32}$$

This can be seen by the replacement $P \to -P$ in eq. (23), which leads to the c-anticyclic analogue of (25), *i.e.*,

$$C'_{jj+p}(\tau) = \tfrac{1}{4}\left\langle \varrho_{\rm ac}\,(\cosh\tau - 2\mathrm{i}\alpha_1\beta_N \sinh\tau)\,(2/\mathrm{i})^p \prod_{k=j}^{j+p-1} (\beta_k\alpha_{k+1})\right\rangle. \qquad (33)$$

Now (32) is obvious from (33) noting that

$$\begin{aligned} \langle \varrho_{\rm ac}\alpha_1\beta_N\rangle &= -\langle \varrho_{\rm c}\alpha_1\beta_N\rangle, \\ \langle \varrho_{\rm ac}\alpha_j\beta_{j-1}\rangle &= \langle \varrho_{\rm c}\alpha_j\beta_{j-1}\rangle \qquad (j = 2, \ldots, N). \end{aligned} \qquad (34)$$

From (32) we have the relations

$$\chi_{\rm ac} = \chi_{\rm c}, \qquad R_{\rm ac}(t) = R_{\rm c}(t). \qquad (35)$$

The susceptibility and the autocorrelation function of M_x in the c-cyclic and c-anticyclic version are equal. Note that this is true even for the finite chain. In general, the properties of the c-cyclic and c-anticyclic XY model are equal only in the thermodynamic limit.

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